

What is claimed is:

1. A method of generating a virtual library of compounds *in silico* comprising:
selecting *in silico* a group of related fragments, each of said fragments constituting a part of said compounds, each of said related fragments having at least one attachment site;
selecting *in silico* at least one further fragment having at least one attachment site; and
linking *in silico* said further fragment to said related fragments by connecting the attachment site of said further fragment to the attachment site of said related fragments to generate said virtual library of compounds.
2. A method of generating a virtual library of compounds *in silico* comprising:
selecting *in silico* a first fragment, said first fragment constituting a part of said compounds and having at least one attachment site;
selecting *in silico* a group of related fragments, each of said group of related fragments having at least one attachment site; and
linking *in silico* each of said group of related fragments to said first fragment by connecting the attachment site of each of said group of related fragments to the attachment site of said first fragment to generate said virtual library of compounds.
3. A method of generating a virtual library of compounds *in silico* comprising:
selecting *in silico* a first group of related fragments, each of said first group of related fragments constituting a part of said compounds and having at least one attachment site;
selecting *in silico* a further group of fragments, each of said further group of fragments having at least one attachment site; and
linking *in silico* each of said first group of related fragments to each of said further group of fragments by connecting the attachment site of each of said first group of related fragments to the attachment site of each of said further group of fragments to generate said virtual library of compounds.
4. The method of claim 1 wherein each of said fragments is introduced *in silico* into said compounds by the use a corresponding reagent.

5. The method of claim 2 wherein each of said fragments is introduced *in silico* into said compounds by the use a corresponding reagent.
6. The method of claim 3 wherein each of said fragments is introduced *in silico* into said compounds by the use a corresponding reagent.
7. A method of identifying *in silico* each compound of a virtual library of compounds comprising:
 - dissecting said compounds into fragments; and
 - identifying each of said fragments in terms of a transformation wherein said transformation is a one to one link between the fragment and a reagent used to introduce said fragment into a compound.
8. The method of claim 7 wherein said transformation is further associated with auxiliary reagents or reaction conditions.
9. A method of generating a virtual library of compounds *in silico* comprising:
 - dissecting said compounds into fragments;
 - representing each of said fragments in silico as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;
 - selecting *in silico* a first group of said fragments, each of said first group of fragments constituting a part of said compounds, each of said first group fragments having at least one attachment site;
 - selecting *in silico* at least one further fragment having at least one attachment site; and
 - linking *in silico* said further fragment to said first group of fragments by connecting the attachment site of said further fragment to the attachment site of said members of said first group of fragments to generate said virtual library of compounds.
10. A method of generating a virtual library of compounds *in silico* comprising:
 - dissecting said compounds into fragments;

representing each of said fragments *in silico* as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;

selecting *in silico* a fragment, said first fragment constituting a part of said compounds, said first fragment having at least one attachment site;

selecting *in silico* a group of further fragments each having at least one attachment site; and

linking *in silico* said group of further fragments to said first fragment by connecting the attachment site of said group of further fragments to the attachment site of first fragment to generate said virtual library of compounds.

11. A method of generating a virtual library of compounds *in silico* comprising:

dissecting said compounds into fragments;

representing each of said fragments *in silico* as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;

selecting *in silico* a first group of said fragments, each of said first group of fragments constituting a part of said compounds, each of said first group fragments having at least one attachment site;

selecting *in silico* a group of further fragments each having at least one attachment site; and

linking *in silico* at least some of the members of said group of further fragments to least some of members of said first group of fragments by connecting the attachment site of the members of said further fragments to the attachment site of said members of said first group of fragments to generate said virtual library of compounds.

12. A method of identifying *in silico* each compound of a virtual library of compounds comprising:

dissecting said compounds into fragments;

adding said fragments together in sequential synthesis rounds; and

tracking the addition of fragments of said compounds.

13. A method of identifying *in silico* each compound of a virtual library of compounds comprising:

- dissecting said compounds into fragments;
- representing each of said fragments in silico as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;
- adding said transformations together in sequential synthesis rounds; and
- tracking transformations in silico.

14. A method of storing information about the member compounds of a virtual library of compounds comprising:

- dissecting each of said compounds into fragments;
- linking together the fragments of each of the compounds; and
- tracking the sequence of linkage for each compound.

15. The method of claim 14 further including:

- grouping two or more compounds of said library together to form a mixture; and
- linking together the tracked information of each of the members of said mixture.

16. The method of claim 14 further including:

- grouping two or more compounds of said library together to form a mixture;
- grouping a further two or more compounds of said library together to form a further mixture;
- linking together the tracked information of each of the members of said mixture; and
- linking together the tracked information of each of the members of said further mixture.

17. A method of storing information about member compounds in a virtual library of compounds comprising:

- dissecting said compounds into fragments;

representing each of said fragments as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;

linking together the transformations of each of the compounds; and
tracking the sequence of linkage for each compound.

18. The method of claim 17 further including:
grouping two or more compounds of said library together to form a mixture; and
linking together the tracked information of each of the members of said mixture.
19. The method of claim 17 further including:
grouping two or more compounds of said library together to form a mixture;
grouping a further two or more compounds of said library together to form a further mixture;
linking together the tracked information of each of the members of said mixture; and
linking together the tracked information of each of the members of said further mixture.
20. The method of claim 17 further including:
defining each said transformation to further include information related to the synthesis of its fragment from its reagent.
21. A method of storing information about the member compounds of a virtual library of compounds comprising:
dissecting each of said compounds into fragments;
grouping two or more compounds of said library together to form a mixture;
linking together the fragments of each of the compounds; and
tracking the sequence of linkage of the members of said mixture.
22. A method of storing information about the member compounds of a virtual library of compounds comprising:

dissecting each of said compounds into fragments;
grouping said compounds of said library into mixtures where each mixture includes two or more member compounds of said library;
linking together the fragments of each of the compounds; and
tracking the sequence of linkage of the members of each said mixture.

23. A method of storing information about the member compounds of a virtual library of compounds comprising:

dissecting each of said compounds into fragments;
representing each of said fragments as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;
grouping two or more compounds of said library together to form a mixture;
linking together the transformation for each of the compounds; and
tracking the sequence of linkage of the members of said mixture.

24. The method of claim 23 further including:

defining each said transformation to further include information related to the synthesis of its fragment from its reagent.

25. A method of storing information about the member compounds of a virtual library of compounds comprising:

dissecting each of said compounds into fragments;
representing each of said fragments as a transformation wherein each transformation is a one to one link between a fragment and a reagent used to introduce said fragment into one of said compounds;
grouping said compounds of said library into mixtures where each mixture includes two or more member compounds of said library;
linking together the transformation for each of the compounds; and
tracking the sequence of linkage of the members of each said mixture.

26. The method of claim 25 further including:
defining each said transformation to further include information related to the synthesis of its fragment from its reagent.